DEVELOPMENT OF A PORT-STREAM BASED EQUATION ORIENTED MODELLING OF DIVIDING WALL COLUMN USING MOSAIC

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Thesis submitted in fulfillment of the requirements
for the award of the degree of
Master of Science

Faculty of Chemical & Natural Resources Engineering

UNIVERSITI MALAYSIA PAHANG

FEBRUARY 2019

ACKNOWLEDGEMENTS

I would like to express my sincere gratitude to my main supervisor Dr.-Ing. Mohamad Rizza Othman who had been guiding and supporting me throughout my research with full of motivation, enthusiasm, and knowledge.

I also would like to express my sincere appreciation to my co-supervisor Dr. Noorlisa Harun for her willingness and guidance in tutoring me for this research.

Furthermore, appreciation to the Malaysia Ministry of Education under grant no. RDU140105 and RDU1603148 for supporting this research work.

Last but not least, special thanks dedicated to my parents for their endless love, support, prayers, and sacrifice.

ABSTRAK

Lajur dinding pembahagian (DWC) dianggap sebagai lajur penyulingan bukan standard yang rumit. Konfigurasi bahagian yang berbeza dalam DWC dibahagikan dengan dinding menegak di dalam ruang meningkatkan kerumitan pemodelan DWC disebabkan kewujudan gelung kitar semula atau aliran yang saling berkaitan. Kaedah yang berorientasikan persamaan (EO) sangat sesuai untuk menangani masalah seperti itu berbanding dengan pendekatan modular berurutan (SM) yang sering membawa kepada masalah penumpuan. Pada tahap yang sangat asas, pendekatan pemodelan DWC perlu dipercayai untuk dilanjutkan sepenuhnya kepada aplikasi lanjutan lain seperti kawalan proses dan pengoptimuman. Dalam makalah ini, pendekatan pemodelan sistematik bagi keadaan mantap DWC dibentangkan yang merangkumi sambungan dan port unit sambungan yang boleh diterima untuk aliran data EO menggunakan MOSAIC. MOSAIC adalah persekitaran pemodelan berasaskan web baru yang direka untuk meminimumkan kesilapan pemodelan, mengurangkan usaha dan kesilapan pengaturcaraan, meningkatkan dokumentasi fail, galakan penyimpanan data koperasi dan perkongsian dan penggunaan semula model dan bahagian model terutamanya untuk pemodelan proses kimia. Pendekatan sedemikian menunjukkan set sistem persamaan yang secara fungsional seperti operasi unit, dengan adanya pelabuhan dan kewujudan aliran dalam menyambungkan semua sistem persamaan bersama-sama. Melalui pendekatan ini, bahagian-bahagian DWC yang berlainan boleh digabungkan sebagai satu lajur dalam satu helaian lajur. Untuk menguji fungsi pendekatan yang dicadangkan, satu kajian kes dengan dua set data eksperimen yang berbeza dipertimbangkan iaitu pemisahan metanol / 1-propanol / 1-butanol. Kemudian model yang dibangunkan digunakan untuk fraksionasi Asid Fatty (FA) untuk memisahkan cahaya (LC), potong tengah (MC), dan potongan berat (HC). Kedua-dua model menunjukkan penumpuan yang baik dengan ralat yang boleh diterima yang membuktikan kesahan pembangunan model. Untuk melanjutkan fungsian model, kajian selanjutnya telah dijalankan untuk menguji analisis interaksi antara pembolehubah yang dimanipulasi (MV) dan pembolehubah terkawal (CV) pada DWC untuk merekabentuk dan mencadangkan konfigurasi kawalan yang sesuai menggunakan analisis nilai tunggal (SVA) dan array gain relatif (RGA).

ABSTRACT

Dividing wall column (DWC) is considered as a complex non-standard distillation column. The different sections configurations within the DWC divided by the vertical wall inside the column increase the complexity of modelling DWC due to the existence of recycle loops or interconnecting streams. An equation-oriented (EO) approach is well suited to handle such problem compared to sequential modular (SM) approach which often leads to convergence problems. At a very basic level, the modelling approach of DWC needs to be reliable to be fully extended to other advanced applications such as process control and optimization. In this paper, a systematic modelling approach of steady-state DWC is presented which encompasses ports and stream unit connectivity that is admissible to EO process flowsheet using MOSAIC. MOSAIC is a new web-based modelling environment which is designed to minimize modelling efforts, minimizing programming efforts, and as a code generator for many programming languages. Such approach present sets of equation system which functionally like a unit operation, with a presence of ports and the existence of streams in connecting all equation systems together. Some adjustment on equations involved has been made accordingly to suit with the port and stream connectivity features particularly in interconnecting streams (liquid and vapour split). Through this approach, different sections of DWC can be combined as a single column in a flowsheet. To test the functionality of the proposed approach, a case study with two different experimental data set were considered which is the separation of methanol/ 1-propanol/ 1-butanol. Then the developed model is applied for the Fatty Acid (FA) fractionation to separate the light-cut (LC), middle-cut (MC), and heavy-cut (HC). Both models show good convergence with an acceptable error below than 10% which proves the validity of the model development.

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LIST OF SYMBOLS

H	Enthalpy
P	Pressure
Q	Heat duty
K	Equilibrium constant/ Open loop gain matrix
D	Distillate flowrate
B	Bottom flowrate
S	Side flowrate
F	Side flowrate
V	Vapour flow /vapour boil-up
L	Liquid flow
c	Interface variable for vapour/liquid composition
f	Interface variable for vapour/liquid flowrate
z	Feed composition
y	Vapour composition/ mole fraction
x	Liquid composition/ mole fraction
α	Liquid split factor
β	Vapour split factor
γ	Activity coefficient

Superscript

V	Vapour
L	Liquid
F	Feed
O	Saturated vapour
D	Distillate
R	Reboiler
bottom	Stripping section
upper	Rectifying section
left	Pre-fractionator section
right	Main section
distillate	Distillate stream product

middle	Middle side stream
in	Flow in
out	Flow out

Subscript

j	j^{th} stage/ controlled variable in RGA
i	j^{th} component/ manipulated variable RGA
k	Interface variable for vapour/liquid composition of component i
o	Reflux rate
D	Distillate
c	Condenser
R	Reboiler
L	Liquid
V	Vapour
W	Bottom

LIST OF ABBREVIATIONS

ACM	Aspen Custom Modeler
AMPL	A Mathematical Programming Language
BDNSOL	Block Decomposition Non-Linear Solver
C++	General Purpose Programming Language
DAEs	Differential Algebraic Equations
DOF	Degree of Freedom
DWC	Dividing Wall Column
EO	Equation Oriented
ES	Equation System
FA	Fatty Acid
Fortran	Formula Translation
FUGK	Fenske-Underwood-Gilliland-Kirkbride
GAMS	General Algebraic Modelling System
gPROMS	General Process Modelling System
GUI	Graphical User Interface
HC	Heavy Cut Component of Fatty Acid Fractionation
LaTeX	Text Document
LC	Light Cut Component of Fatty Acid Fractionation
MathML	Mathematical Markup Language
MESH	Material, Equilibrium, Summation, Heat
MC	Middle Cut Component of Fatty Acid Fractionation
MIMO	Multiple-Input Multiple-Output
MOSAIC	Model Specification on Documentation Level
NLE	Non-Linear Equation System
NDOF	Number degree of freedom
NEQN	Number of equations
NFIX	Number of fixed variables
NSPEC	Net specifications
NVAR	Number of variables
OCM	Oxidative Coupling of Methane
ODE	Ordinary Differential Equations

RADFRAC	ASPEN’s Rigorous Distillation Method
RGA	Relative Gain Array
SCILAB	Numerically Oriented Programming Language
SISO	Single-Input Single-Output
SM	Sequential Modular
SPARSE	Newton-Type Method Without Block Decomposition

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